

# Equation of motion approach to the solution of Anderson model

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Based on an equation of motion approach the single impurity Anderson model(SIAM) is reexamined. Using the cluster expansions the equations of motion of Green functions are transformed into the corresponding equations of motion of connected Green functions, which provides a natural and uniform truncation scheme. A factor of two missing in the Lacroix's approximation for the Kondo temperature is gained in the next higher order truncation beyond Lacroix's. A quantitative improvement in the density of states at the Fermi level is also obtained.

The single impurity Anderson model(SIAM)<sup>1</sup> is one of the most fundamental and probably best understood models in the field of strongly correlated electronic systems. It was proposed to describe the properties of magnetic impurities in non-magnetic metallic hosts (for a review see e.g. Ref. 2). Yet, the SIAM has been used widely to imitate mixed valence and heavy fermion systems.<sup>3-6</sup> Since the SIAM was proposed, a variety of standard techniques have been applied to it and new methods have been developed to study its static and dynamical properties, basically in the whole parameter space. ( For a recent review see, e.g. Ref. 7.)

The method of equations of motion(EOM) of Green functions(GFs) is one of the most important tools to solve the model Hamiltonian problems in condensed matter physics. One of its most appealing features is that it can work in the whole parameter space. Many authors have applied the EOM approach to the SIAM for finite  $U^{1,8,9}$  or infinite  $U^{10-14}$ . In order to close the chain of equations it is usual to introduce the conventional Tyablikov decoupling scheme.<sup>15</sup> Lacroix employed thus decoupling scheme for higher order GFs.<sup>12,13</sup> In the limit of strong intra-atomic Coulomb interaction he did not get the correct expression of Kondo temperature from his high- and/or intermediate-temperature solutions<sup>12</sup> at his approximation level.

In the present paper we shall go beyond Lacroix's approximation in a slightly different way. In the following we use the correlation dynamics approach<sup>17</sup> to treat the problem. After writting down the hierarchy of EOM of the GFs the Tyablikov decoupling scheme is not applied directly. Instead systematic cluster expansions are employed, which express the higher order GFs in terms of same order connected GFs and lower order GFs, the hierarchy of EOM of the usual GFs is thus transformed

into that of EOM of the connected GFs. The connected GFs are defined such that they can not be reduced to the low order ones by any way of decoupling. The hierarchy of equations of the connected GFs provides a natural and uniform truncation scheme. Our formalism, which is essentially equivalent to the Tyablikov decoupling scheme, is more systematic. The well known results like mean field theory,<sup>1</sup> Hubbard-I approximation,<sup>11</sup> two-peak solutions,<sup>16</sup> and Lacroix's results<sup>12,13</sup> are recovered exactly in successively higher levels of truncation. To go beyond Lacroix we introduce even higher order truncation. The Kondo temperature obtained is in agreement with the exact one<sup>18</sup> except for a prefactor. The density of states(DOS) of the SIAM is calculated numerically at finite temperature. A quantitative improvement on the DOS at the Fermi level is also obtained.

Consider the Hamiltonian of the conventional SIAM<sup>1</sup>

$$H = \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \varepsilon_d \hat{n}_{d\sigma} + \frac{1}{2} U \sum_{\sigma} \hat{n}_{d\sigma} \hat{n}_{d\bar{\sigma}} + V \sum_{k\sigma} (c_{k\sigma}^+ d_{\sigma} + d_{\sigma}^+ c_{k\sigma}). \quad (1)$$

The notation used is as usual. In this paper the DOS for conduction electrons is taken to be a constant,  $\rho(\varepsilon) = \frac{1}{2D}$  as  $-D < \varepsilon < D$ . The width of the virtual bound state is  $\Delta = \pi \langle V^2 \rangle / (2D)$ .<sup>1</sup>

Using the Zubarev notation<sup>15</sup>  $G_{A,B}(\omega) = \ll A; B \gg$ , it is straightforward to write down the EOM for the one-particle GFs

$$\left( \omega - \varepsilon_d - \sum_k \frac{V^2}{\omega - \varepsilon_k} \right) \ll d_{\sigma}; d_{\sigma}^+ \gg = 1 + U \ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg, \quad (2)$$

and for the high order GFs

$$\begin{aligned} (\omega + \varepsilon_d - \varepsilon_{k'} - \varepsilon_k) \ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg = \\ -U \ll \hat{n}_{d\sigma} d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg + V (\ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg \\ + \ll \hat{n}_{d\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg - \sum_{k''} \ll c_{k''\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg), \end{aligned} \quad (3a)$$

$$\begin{aligned} (\omega + \varepsilon_{k'} - \varepsilon_d - \varepsilon_k) \ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg = \\ U \ll \hat{n}_{d\sigma} c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg + V (\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg \\ - \ll \hat{n}_{d\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg + \sum_{k''} \ll c_{k''\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg), \end{aligned} \quad (3b)$$

$$(\omega + \varepsilon_{k'} - \varepsilon_k - \varepsilon_d) \ll c_{k'\bar{\sigma}}^+ c_{k\sigma} d_{\sigma}; d_{\sigma}^+ \gg = \langle c_{k'\bar{\sigma}}^+ c_{k\sigma} \rangle$$

$$+U \ll \hat{n}_{d\bar{\sigma}} c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg + V (\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg - \ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg + \sum_{k''} \ll c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} c_{k''\sigma}; d_{\sigma}^+ \gg). \quad (3c)$$

To save space, the EOM for the high order GFs  $\ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg$ ,  $\ll \hat{n}_{d\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg$ ,  $\ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg$ , and  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg$  are omitted. One can find their EOM in Ref. 12. Instead of employing directly the Tyablikov decoupling scheme, we make use of a cluster expansions to separate the connected part of the GFs. As an example, the high order GF  $\ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg$  is expressed as follows:

$$\ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg = n_{d\bar{\sigma}} \ll d_{\sigma}; d_{\sigma}^+ \gg + \ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c, \quad (4)$$

where  $\ll \dots \gg_c$  represents a connected GF and  $n_{d\bar{\sigma}} = \langle \hat{n}_{d\bar{\sigma}} \rangle$ . It is straightforward to derive the EOM for the connected GFs. We write down the first two as follows:

$$\left( \omega - \varepsilon_d - U n_{d\bar{\sigma}} - \sum_k \frac{V^2}{\omega - \varepsilon_k} \right) \ll d_{\sigma}; d_{\sigma}^+ \gg = 1 + U \ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c, \quad (5a)$$

$$[\omega - \varepsilon_d - U(1 - n_{d\bar{\sigma}})] \ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c = U n_{d\bar{\sigma}} (1 - n_{d\bar{\sigma}}) \ll d_{\sigma}; d_{\sigma}^+ \gg + V \sum_k (\ll \hat{n}_{d\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c + \ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c - \ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c). \quad (5b)$$

It is not difficult to obtain the EOM of the other connected GFs such as  $\ll \hat{n}_{d\sigma} c_{k\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ , and  $\ll c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c$ .

In the following we discuss briefly the solutions at different orders of approximation. The lowest order truncation, i.e.  $\ll \hat{n}_{d\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c \approx 0$ , leads to the mean field theory, while next higher order truncation, namely,  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c \approx 0$ ,  $\ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c \approx 0$ , and  $\ll \hat{n}_{d\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c \approx 0$ , corresponds to Hubbard-I approximation. Subsequently, the solution with two peaks localized at  $\varepsilon_d$  and  $\varepsilon_d + U$  with weights  $1 - n_{d\bar{\sigma}}$  and  $n_{d\bar{\sigma}}$  respectively, can be obtained from the truncation  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c \approx 0$ ,  $\ll d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c \approx 0$ ,  $\ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c \approx 0$ , and  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c \approx 0$ . To reach Lacroix's approximation,<sup>12</sup> the connected GFs like  $\ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ , and  $\ll c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c$  involving two conduction electrons are neglected. After some algebraic manipulation the GF  $\ll d_{\sigma}; d_{\sigma}^+ \gg$  in the limit of  $U \rightarrow \infty$  reads

$$\ll d_{\sigma}; d_{\sigma}^+ \gg = \left( 1 - n_{d\sigma} - V \sum_k \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} \right) (\omega - \varepsilon_d + i\Delta - V^2 \sum_{k,k'} \frac{\langle c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} + \sum_{k'} \frac{V^3}{\omega - \varepsilon_{k'}} \sum_k \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k})^{-1}. \quad (6)$$

Eq.(6) recovers exactly Lacroix's results. We shall discuss in detail the solution of eq.(6) together with the solutions of the next order approximation.

To go beyond the Lacroix's approximation it is necessary to consider the EOM of the connected GFs  $\ll d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ ,  $\ll c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma}; d_{\sigma}^+ \gg_c$ , and  $\ll c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} d_{\sigma}; d_{\sigma}^+ \gg_c$ , and to assume higher order correlation Green's functions to be zero. After a lengthy but straightforward calculation,  $\ll d_{\sigma}; d_{\sigma}^+ \gg$  is obtained finally as

$$\ll d_{\sigma}; d_{\sigma}^+ \gg = \frac{1 - n_{d\bar{\sigma}} - V \sum_k \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} - \delta}{\omega - \varepsilon_d + i\Delta - \sum_{k,k'} \frac{V^2 \langle c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} + \gamma}, \quad (7)$$

with

$$\delta = \frac{V^2}{n_{d\sigma}} \sum_k \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} \sum_{k'} \frac{\langle d_{\sigma}^+ c_{k'\sigma} \rangle}{\omega - \varepsilon_{k'}}, \quad (8a)$$

$$\gamma = -i\Delta\delta + \beta + 2 \sum_{k,k'} \frac{V^3 \langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle}{(\omega - \varepsilon_k)(\omega - \varepsilon_{k'})} + \frac{V^2}{n_{d\bar{\sigma}}} \sum_{k,k'} \frac{(\langle \hat{n}_{d\bar{\sigma}} c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle_c - \langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} \rangle)}{\omega - \varepsilon_k} - \frac{V^3}{n_{d\sigma}} \sum_{k,k',k''} \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle c_{k'\bar{\sigma}}^+ c_{k''\sigma} \rangle + \langle \hat{n}_{d\sigma} d_{\sigma}^+ c_{k'\sigma} \rangle}{(\omega - \varepsilon_k)(\omega - \varepsilon_{k'})} + \frac{V^2}{n_{d\sigma}} \sum_{k,k'} \frac{\langle d_{\bar{\sigma}}^+ d_{\sigma}^+ c_{k'\bar{\sigma}} c_{k\sigma} \rangle - \langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle d_{\sigma}^+ c_{k'\sigma} \rangle}{\omega - \varepsilon_k}, \quad (8b)$$

where

$$\beta = \frac{V^2}{n_{d\sigma}} \sum_{k,k'} \frac{\langle d_{\bar{\sigma}}^+ d_{\sigma}^+ c_{k'\bar{\sigma}} c_{k\sigma} \rangle_c - \langle d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma} \rangle_c}{\omega - \varepsilon_k}. \quad (8c)$$

In the above derivation, we have used the Hermitian conditions like  $\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle = \langle c_{k\bar{\sigma}}^+ d_{\bar{\sigma}} \rangle$ , etc. To simplify the solution and to obtain some analytical results, we notice the following facts: (i)  $\langle d_{\bar{\sigma}}^+ d_{\sigma}^+ c_{k'\bar{\sigma}} c_{k\sigma} \rangle \sim 0$  and  $\langle \hat{n}_{d\sigma} d_{\sigma}^+ c_{k\sigma} \rangle \sim 0$  in the limit of  $U \rightarrow \infty$ , in which doubly occupied states are unfavorable. (ii)  $\langle \hat{n}_{d\bar{\sigma}} c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle$  is a new correlation function related to  $\langle d_{\bar{\sigma}}^+ \hat{n}_{d\bar{\sigma}} c_{k\bar{\sigma}} \rangle$  by the EOM and the spectral theorem. From observation (i) it is evident  $\langle d_{\bar{\sigma}}^+ \hat{n}_{d\bar{\sigma}} c_{k\bar{\sigma}} \rangle \sim 0$ . Thus, the spectral theorem implies that  $\langle c_{k'\bar{\sigma}}^+ \hat{n}_{d\bar{\sigma}} c_{k\bar{\sigma}} \rangle \sim 0$ . The cluster expansion yields simply  $\langle \hat{n}_{d\bar{\sigma}} c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle_c - \langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} \rangle \sim -n_{d\bar{\sigma}} \langle c_{k'\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle$ . (iii)  $\beta$  contains two higher order equal time correlations. One is the double hopping correlation  $\langle d_{\bar{\sigma}}^+ d_{\sigma}^+ c_{k'\bar{\sigma}} c_{k\sigma} \rangle_c$  which is approximately equal to  $-\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle d_{\sigma}^+ c_{k'\sigma} \rangle$  based on observation (i). The other is the spin-flip correlation  $\langle d_{\bar{\sigma}}^+ c_{k'\bar{\sigma}}^+ d_{\bar{\sigma}} c_{k\sigma} \rangle_c$ , which should be calculated self-consistently. For simplicity, we just assume this correlation to be zero. Thus, we have approximately

$$\beta \sim -\frac{V^2}{n_{d\sigma}} \sum_{k,k'} \frac{\langle d_{\bar{\sigma}}^+ c_{k\bar{\sigma}} \rangle \langle d_{\sigma}^+ c_{k'\sigma} \rangle}{\omega - \varepsilon_k}.$$

iv) By using the spectral theorem again, it is easy to show that  $\sum_{k'} V \langle d_{\sigma}^{\dagger} c_{k'\sigma} \rangle = -i\Delta n_{d\sigma}$ .

Based on the above observations we obtain finally

$$\begin{aligned} \ll d_{\sigma}; d_{\sigma}^{\dagger} \gg = & \left( 1 - n_{d\sigma} - \sum_k \frac{V \langle d_{\sigma}^{\dagger} c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} - \delta \right) \\ & \times (\omega - \varepsilon_d + i\Delta(1 - \delta) - 2 \sum_{k,k'} \frac{V^2 \langle c_{k'\bar{\sigma}}^{\dagger} c_{k\bar{\sigma}} \rangle}{\omega - \varepsilon_k} \\ & - \frac{1}{n_{d\sigma}} \sum_{k,k',k''} \frac{V^3 \langle d_{\sigma}^{\dagger} c_{k\bar{\sigma}} \rangle \langle c_{k''\bar{\sigma}}^{\dagger} c_{k'\sigma} \rangle}{(\omega - \varepsilon_k)(\omega - \varepsilon_{k'})})^{-1}, \end{aligned} \quad (9)$$

where  $\delta$  is given by eq. (8a).

The average functions  $\langle c_{k'\bar{\sigma}}^{\dagger} c_{k\bar{\sigma}} \rangle$ ,  $\langle c_{k''\bar{\sigma}}^{\dagger} c_{k'\sigma} \rangle$  and  $\langle d_{\sigma}^{\dagger} c_{k\bar{\sigma}} \rangle$  have to be calculated self-consistently. To distinguish our results for  $\ll d_{\sigma}; d_{\sigma}^{\dagger} \gg$  from Lacroix's we use  $G_d^L(\omega + i\eta)$  for the Lacroix's solution and  $G_d^N(\omega + i\eta)$  for our solution. Following Lacroix, eq. (6) reads<sup>12</sup>

$$G_d^L(\omega + i\eta) = \frac{1 - n_d - A(\omega + i\eta)}{\omega - \varepsilon_d + i\Delta + B(\omega + i\eta) - 2i\Delta A(\omega + i\eta)}, \quad (10)$$

where

$$A(\omega + i\eta) = -\frac{\Delta}{\pi} \int d\omega' f(\omega') \frac{(\ll d_{\sigma}; d_{\sigma}^{\dagger} \gg)^*}{\omega' - \omega - i\eta}, \quad (11a)$$

$$B(\omega + i\eta) = \frac{\Delta}{\pi} \int d\omega' \frac{f(\omega')}{\omega' - \omega - i\eta}. \quad (11b)$$

Similarly, the eq.(9) becomes

$$\begin{aligned} G_d^N(\omega + i\eta) = & (1 - n_d - A - \frac{A^2}{n_d})[\omega - \varepsilon_d + i\Delta(1 - \frac{A^2}{n_d}) \\ & + 2(B - i\Delta A) + \frac{A}{n_d}(B - i\Delta A)]^{-1}. \end{aligned} \quad (12)$$

For the sake of simplicity, we have considered the non-magnetic case, i.e.  $n_{d\uparrow} = n_{d\downarrow} = n_d$  which is half of the total d-electron number  $n_t$ . By the spectral theorem:

$$n_t = \int f(\omega') \rho(T, \omega') d\omega', \quad (13)$$

where  $\rho(T, \omega) = -\frac{2}{\pi} \text{Im} G_d(\omega + i\eta)$  is the DOS with finite temperature and  $f(\omega) = \frac{1}{\exp[(\omega - E_F)/T + 1]}$  is Fermi distribution function.

Eqs.(12) and (10) with (13) constitute two sets of self-consistent equations respectively. They can be solved numerically. Before performing the numerical calculation we simply consider its analytic solutions in the high and low temperature limits.

At high temperature  $A(\omega + i\eta)$  is a small correction and thus an expansion with respect to  $\Delta$  is available. After some algebra, one obtains the Kondo temperature

$$T_k = D \exp \frac{\pi(\varepsilon_d - E_F)}{\Delta}, \quad (14)$$

for the Lacroix's solution, and

$$T_k = D \exp \frac{\pi(\varepsilon_d - E_F)}{2\Delta}, \quad (15)$$

for our solution. Comparing with the exact expression obtained by Haldane<sup>18</sup>

$$T_k \approx (D\Delta)^{1/2} \exp \frac{\pi(\varepsilon_d - E_F)}{2\Delta}, \quad (16)$$

our result is evidently an improvement. It is also helpful to check the low temperature result. At low temperature limit, as Lacroix noticed,  $A(\omega + i\eta)$  must be large, especially as  $\omega$  is near the Fermi level. We consider the zero temperature case. In this case,  $A, B$  can be written as

$$A(\omega + i\eta) = -\frac{\Delta}{\pi} G_d^*(\omega) \left( \frac{i\pi}{2} + \ln \frac{|\omega - E_F|}{D} \right), \quad (17a)$$

$$B(\omega + i\eta) = \frac{\Delta}{\pi} \left( \frac{i\pi}{2} + \ln \frac{|\omega - E_F|}{D} \right). \quad (17b)$$

Inserting  $A$  and  $B$  into the Eq.(12), one obtain readily

$$G_d^N(E_F) = \frac{\Delta}{\pi} \frac{G_d^{N*}(E_F)}{2i\Delta^2/\pi G_d^{N*}(E_F) + \Delta/\pi}. \quad (18)$$

The expression is exactly the same as that obtained by Lacroix.<sup>12</sup>

In the following we solve numerically the DOS by the self-consistent equations (12) and (13) in the Kondo regime. The following parameters are considered. The total number of the d-electron is taken to be 0.9, which determines self-consistently the chemical potential. The halfwidth  $D$  is assumed to be 1, which defines the energy scale. The d-electron level  $\varepsilon_d$  is taken to be 0 and the width of the virtual bound state  $\Delta = 0.01D$ . In Fig. 1 the DOS for our solution (solid line) is shown at the very low temperature  $T = 10^{-5}\Delta$ . For comparison the DOS for the solution (10) with the above parameters (dash line), which is not available in Ref. 13, is also presented. In two cases the lorentzian resonance peaks are slightly shifted. In the Kondo regime better behaviors including larger  $|\varepsilon_d - E_F|$  and a more pronounced Kondo peak are observed in our solution. A good test for the DOS is provided by the Friedel sum rule,<sup>19</sup> which relates the DOS at the Fermi level to the occupation number  $n_t$  at  $T = 0$  K, i.e.  $\rho(T = 0, E_F) = \frac{1}{\pi\Delta} \sin^2(\frac{\pi n_t}{2})$ .<sup>20</sup> This value is about 31 using the above parameter values. Our result of about 25 is in rough agreement with this exact value, while agreement is not as good for Lacroix's approximation.

The temperature dependence of the DOS at the Fermi level is plotted in Fig. 2 in the regime of the Kondo temperature, which is given by eq. (15) in our calculation. It is evident that our result is comparable to the numerical renormalization group(NRG) result(dotted line).<sup>20</sup> The result(dash line) from the Lacroix's approximation[eq.(10)] with the same parameters above is far

below the NRG results. Therefore, the higher order correlation effects can not be neglected in describing the system properties quantitatively.

In conclusion, by using the EOM for the connected GFs we obtained the solution of the SIAM beyond Lacroix's approximation. The missing factor of two in the expression of Kondo temperature in Lacroix's approximation is regained, which is in agreement with the exact one except for a prefactor. The DOS and its temperature dependence at the Fermi level are obtained numerically. A quantitative improvement on Lacroix's approximation is found, which shows that the higher order correlation effects are important for describing the system properties quantitatively.

**Acknowledgements** This work was supported in part by the Deutscher Akademischer Austauschdienst (DAAD), and by the National Natural Science Foundation, the Doctoral Education Fund of Education Ministry, and the Nuclear Theory Research Center of HIRFL of China.

this reference.

- <sup>21</sup> The temperature dependence of the DOS at the Fermi level was presented in Ref. 13. But the author used the parameter  $\frac{E_0 - E_F}{D} = 0.1$  ( $E_0$  is the d-electron level), which does not describe the Kondo regime; according to Ref. 20, his parameters describe the mixed valence or empty orbital regime.

FIG. 1. DOS for our solution (solid line) and for the Lacroix's approximation (dash line) at  $T = 10^{-5}\Delta$ . The values of the parameters are  $n_d = 0.9$ ,  $\varepsilon_d = 0.0$ ,  $\Delta = 0.01D$ , and  $D = 1$ . The d-electron level and the position for the Fermi level are indicated by the arrows.

FIG. 2. Temperature dependence of  $\rho(T, E_F)$ . The parameters except the temperature are the same as those given in Fig. 1

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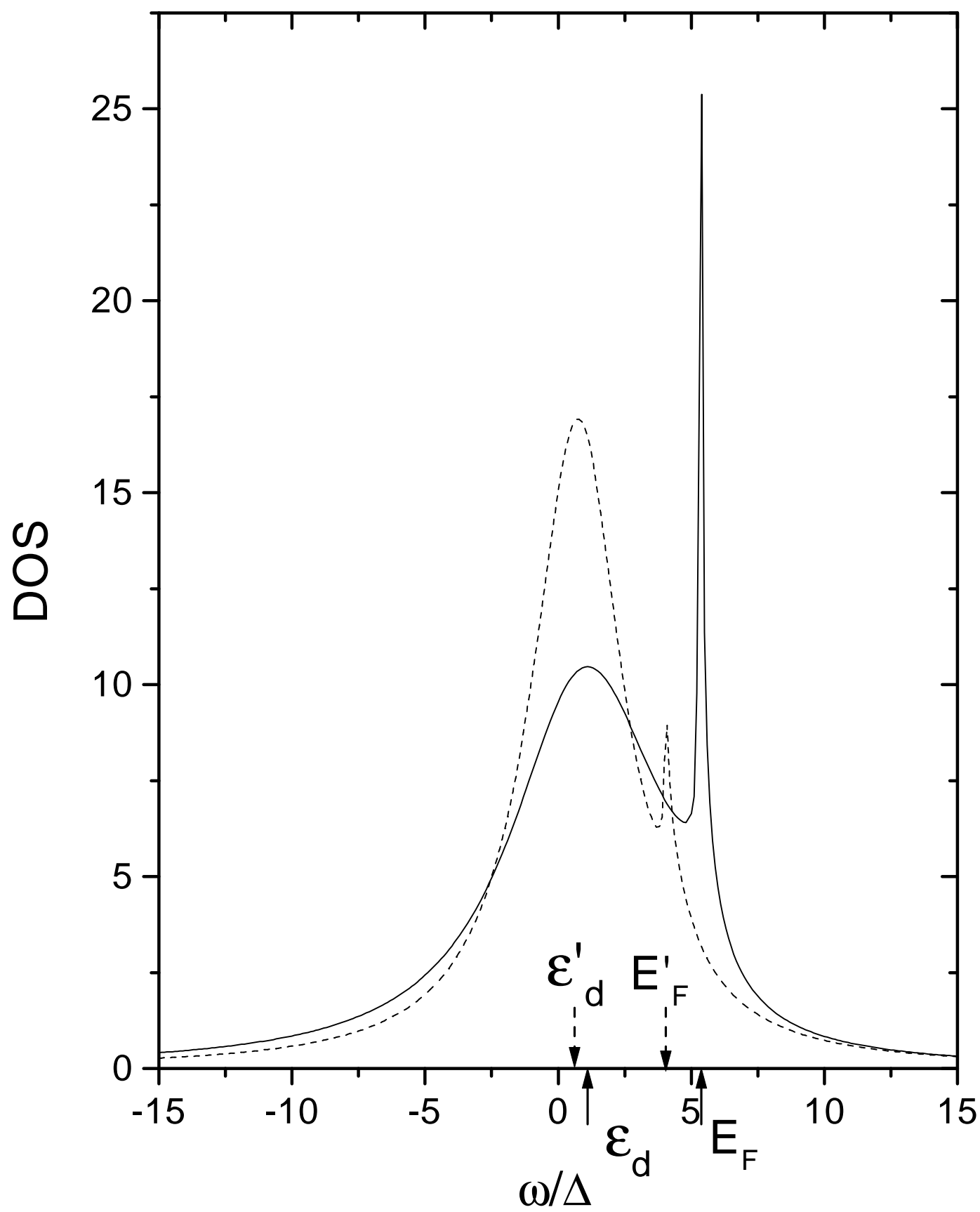
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<sup>18</sup> F.D.M. Haldane, Ph. D. thesis, University of Cambridge, 1978; Phys. Rev. Lett. **40**, 416 (1978).

<sup>19</sup> F. Friedel, Phil. Mag. **43**, 153 (1952).

<sup>20</sup> T.A. Costi, A.C. Hewson and V. Zlatić, J. Phys.: Condens. Matter **6**, 2519 (1994). The data are read from Fig. 7 in

Luo *et al*, Fig.1



Luo *et al*, Fig. 2

